

DERIVATION OF A TWO-PHASE FLOW MODEL ACCOUNTING FOR SURFACE TENSION

Hélène Mathis

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DERIVATION OF A TWO-PHASE FLOW MODEL ACCOUNTING FOR SURFACE TENSION

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ABSTRACT. This paper addresses the derivation of a two-phase flow model accounting for surface tension effects, by means of the Stationary Action Principle (SAP). The Lagrangian functional, defining the Action, is composed of a kinetic energy, accounting for interface feature, and a potential energy. The key element of the model lies on the assumption that the interface separating the two phases admits its own internal energy, satisfying a Gibbs form including both surface tension and interfacial area. Thus surface tension is taken into account both in the potential energy and the kinetic one which define the Lagrangian functional. Applying the SAP allows to build a set of partial differential equations modelling the dynamics of the two-phase flow. It includes evolution equations of the volume fraction and the interfacial area, accounting for mechanical relaxation terms. The final model is shown to be well posed (hyperbolicity, Lax entropy).

Key-words. Two-phase compressible flows, interfacial area, thermodynamics, Stationary Action Principle, hyperbolicity

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1. INTRODUCTION

The modelling of compressible multiphase flows have been the topic of a large literature over the past decades, notably for practical applications such as nuclear safety of pressurized water reactor. In the context of the loss of coolant accident for instance, the liquid water refrigerant is submitted to high pressure and temperature condition, so that a break in the refrigerant circuit could lead to the appearance of vapor and induce shock and phase transition waves [1]. Hence the question is not only to capture the wave structure but also to get informations on the different exchanges occuring at the liquid-vapor interface.

These transfers depend strongly on the area of the interfaces, even when focusing on the large scale description. Several approaches have been proposed to establish the evolution of the interfacial area, depending mostly of the scale of description. When focusing on polydisperse flows, with many inclusions, bubbles or droplets, the modelling of the bubbles pulsation requires to keep a small scale description. For instance in [29], the author proposes a transport equation based on heuristics of particulate suspensions, assuming that both phases evolve with distinct velocities. Then focusing on the small scale, he proposes a second transport equation while studying the fluctuations of a small interface element. Following this approach several models have been proposed in a serie of works [8, 7, 6, 9], considering the one-velocity framework. The set of bubbles/droplets is described by a probability density function, which satisfies the so-called Williams-Boltzmann equation. The distribution function describes then the probability of presence of a bubble at a certain time and position, which evolves with a given velocity. It also takes into account topological properties of the bubble/droplet such as its volume or radius. In a recent contribution [30], the authors propose to make the density distribution depend on topological informations of the interface as well, considering in particular the level set of the interface and its local mean curvature. Doing so they manage to get informations on the interfacial area and provide a full partial differential equations (PDEs) model for the mixture dynamics, by means of Stationary Action Principle (SAP) applied to a given Lagrangian functional. Note that the model they get enters the class of averaged models, in the sense that it does not provide any information on the topology of the interface, which is solely indicated by evolution equations of 1) the void fraction of one of the two phases and 2) the interfacial area.

In the application we have in mind, a precise description of the interface topology is not mandatory. The high heterogeneity of the flows, the strong temperature and pressure conditions suggest to consider averaged models where the interface is depicted implicitly. However the interface between the two phases is the locus of all the thermodynamical exchanges, and the relaxation towards the thermodynamical depends strongly on this area, especially the relaxation time scales. This is the approach adopted in [3] where a convection equation of the interfacial area is coupled to a barotropic three-phase flow model of Baer-Nunziato type. The equation is endowed with a source term which cancels as soon as the Weber number (ratio of the momentum over the surface tension) is greater than a given threshold or when the relative velocity of the two phases is null. The interfacial area equation is inspired by the modelling proposed in [31] for steam explosion simulations.

In the latter references the surface tension effect solely depends on geometrical features which define the kinetic energy of the bulk and the interface. In all the proposed derivations, the thermodynamic behaviour of the interface is not considered, and in particular, the surface tension does not affect the potential energy of the system. This is precisely this point of vue that we are developing here.

The derivation of the averaged fluid-interface model is obtained adapting the Stationary Action Principle as detailled in [4]. The core of our model relies on the rigorous derivation of the potential energy involved in the Lagrangian functional, while the kinetic energy accounts for smale scales, in the spirit of [8].

The originality of our approach is to consider the surface tension not only as a dynamical feature but also a thermodynamics one. To do so we come back to classic extensive thermodynamics in the sense of Gibbs [5, 27] to described as rigorously as possible the thermodynamical behaviour of the fluid-interface system. In the case of two phase flows, this methodology has been used for instance in [22, 21, 12, 13] and in the quoted references, leading to thermodynamically consistent multiphase flow models (for immiscible and miscible mixtures). The novelty here relies in the fact that the interface is assumed to be described by an extensive internal energy function, assuming that the interface has no mass, occupies no volume but is characterized by its internal energy which satisfies a Gibbs form involving not only temperature/entropy but also surface tension/interfacial area variations. Note that this characterization goes back to [28, 27] and more recently in [32] to model (multiphase) flows in porous media.

The paper is organized as follows. The Section 2 is devoted to the thermodynamical modelling focusing on the extensive and intensive descriptions of the two phases and the interface. The internal energy of the fluid-system is defined and the associated mixture temperature, pressure and chemical potential as well. Besides the initial setting ensures that the interfacial area and the surface tension appear naturally in the pressure. When focusing on the characterization of the thermodynamical equilibrium, some interessant properties arise, especially the fact that the mechanical equilibrium is depicted by a differential form involving the volume fraction and the interfacial area.

In Section 3 we make use of the fluid-interface internal energy to define the potential energy of the Lagrangian functional defining the Action. A review of the so-called small scale kinetic energies available in the literature is presented and motivates the choice of our kinetic energy. Then the SAP leads to the obtention of a set of PDEs describing the dynamics of the fluid-interface system. Since the SAP qualifies reversible processes, it guarantees the conservations of the momentum and the total energy and the hyperbolicity and symmetrization property of the model. Such properties are given in Section 4.

2. Thermodynamical modelling

We consider the fluid-interface system with volume V, mass M and entropy S. It is composed of the two immiscible fluids or phases k = 1, 2 with indices k = 1, 2, separated by an interface, with index i. At each point of this system, local equilibrium is reached so that each part of the system is depicted by its own Equation of State (EoS). In the present section are listed the notations and assumptions for the fluid phases and the interface, both in extensive and intensive variables. Then, the second law of thermodynamics allows us to characterize the fluid-interface internal energy and the thermodynamical equilibrium of the system.

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2.1. Fluid phases. A phase k = 1, 2 of volume $V_k \ge 0$, entropy $S_k \ge 0$ and mass $M_k \ge 0$ is entirely described by its extensive internal energy function E_k which complies with the following assumptions:

- $(M_k, V_k, S_k) \mapsto E_k(M_k, V_k, S_k)$ is \mathcal{C}^2 on $(\mathbb{R}_+)^3$,
- $(M_k, V_k, S_k) \mapsto E_k(M_k, V_k, S_k)$ is convex,
- $\forall \lambda \in \mathbb{R}^*_+, \forall (M_k, V_k, S_k) \in (\mathbb{R}_+)^3, E_k(\lambda M_k, \lambda V_k, \lambda S_k) = \lambda E_k(M_k, V_k, S_k).$

The last assumption corresponds to the extensive character of the internal energy function : when doubling the volume, mass and entropy of the system, the extensive internal energy is doubled as well. This homogeneity property implies that the extensive internal energy E_k is convex but not strictly convex.

Some intensive parameters are defined as partial derivatives of E_k :

- the pressure $p_k(M_k, V_k, S_k) = -\partial E_k / \partial V_k(M_k, V_k, S_k)$,
- the temperature $T_k(M_k, V_k, S_k) = \partial E_k / \partial S_k(M_k, V_k, S_k) > 0$,
- the chemical potential $\mu_k(M_k, V_k, S_k) = \partial E_k / \partial M_k(M_k, V_k, S_k)$,

leading to the total differential form

(1)
$$\mathrm{d}E_k = T_k \mathrm{d}S_k - p_k \mathrm{d}V_k + \mu_k \mathrm{d}M_k,$$

referred as extensive (phasic) Gibbs form in the sequel. Since the internal energy is extensive, its satisfies the Euler relation

(2)
$$E_k = T_k S_k - p_k V_k + \mu_k M_k.$$

Some intensive variables and potentials can be defined while considering the extensive ones relatively to the mass of the phase k. We introduce the specific volume $\tau_k = V_k/M_k$ and the specific entropy $s_k = S_k/M_k$ of the phase k = 1, 2. Then the specific internal energy $e_k(\tau_k, s_k)$ corresponds to a restriction of the extensive energy:

(3)
$$e_k(\tau_k, s_k) = E_k(1, \tau_k, s_k).$$

The phasic pressure and temperature can be defined as functions of the intensive variables as well (while keeping the same notations):

(4)
$$p_k(\tau_k, s_k) = -\partial e_k / \partial \tau_k(\tau_k, s_k), \quad T_k(\tau_k, s_k) = \partial e_k / \partial s_k(\tau_k, s_k).$$

The intensive potentials comply thus with an intensive differential (phasic) Gibbs form:

(5)
$$\mathrm{d}e_k = T_k \mathrm{d}s_k - p_k \mathrm{d}\tau_k.$$

Note that scaling the extensive Euler relation (2) with respect to the mass M_k gives another definition of the chemical potential μ_k , which turns to be the Legendre transform of the internal energy e_k :

(6)
$$\mu_k = e_k - T_k s_k + p_k \tau_k.$$

2.2. The interface. The interface separating the two phases is supposed to be sharp and to have no volume and no mass. Adopting an extensive description, it is thus characterized by its energy E_i , function of its entropy S_i and its area A_i . According to the first principle of thermodynamics, it holds

(7)
$$dE_i = T_i dS_i + \gamma_i dA_i,$$

where $\gamma_i(S_iA_i)$ is the surface tension and $T_i(S_i, A_i)$ the interfacial temperature. The internal energy E_i being an extensive quantity, its complies with the Euler relation

(8)
$$E_{\rm i} = T_{\rm i}S_{\rm i} + \gamma_{\rm i}A_{\rm i}$$

which yields, after differentiating and subtracting (7), the so-called Gibbs–Duhem relation

(9)
$$0 = S_{i} dT_{i} + A_{i} d\gamma_{i}.$$

Since the interface has no mass, a way to deduce intensive potentials is to scale with respect to the volume V of the fluid-interface system. This way we introduce the interfacial density area

(10)
$$a_{\rm i} = A_{\rm i}/V,$$

while scaling the area A_i by the volume V of the mixture.

Now, scaling the extensive variables with respect to the interface area A_i defines the interfacial intensive entropy $s_i = S_i/A_i$ and the interfacial intensive energy $e_i = E_i/A_i$. Scaling the Euler relation (8) with respect to the volume V of the mixture, one deduces

(11)
$$e_{i} = T_{i}s_{i} + \gamma_{i},$$

and doing so with the interfacial Gibbs relation (7) gives

(12)
$$e'_{i}(s_{i}) = T_{i}$$

and

(13)
$$d(a_i e_i) = T_i d(a_i s_i) + \gamma_i da_i.$$

By the definition (10) of the interfacial density area a_i , observe that the relation (9) gives

(14)
$$\gamma_i'(T_i) = -s_i(T_i)$$

This derivative relation is not often mentioned in the literature, but it can be found in [28, 27] for instance.

2.3. Thermodynamical equilibrium. We now consider the fluid system with volume V, mass M and entropy S. The two immiscible phases k = 1, 2 are separated by the interface of area A_i . Accounting for the constitutive laws of the two fluid phases and the interface, we now turn to the characterization of thermodynamical equilibrium of the whole system. For a given state (M, V, S, A_i) of the system, different modelling constraints have to be set. As mentioned before, the two phases are supposed to be immiscible and that no vacuum appears, such that the total volume is the sum of the phasic volumes

(15)
$$V = V_1 + V_2,$$

since the interface has no volume. As the mass conservation of the system is concerned, it holds

$$(16) M = M_1 + M_2$$

since the interface has no mass and only mass transfer can occur between the two phases (and not with the interface). Finally the homogeneity property of the system entropy states that

(17)
$$S = S_1 + S_2 + S_i.$$

It is convenient to provide the intensive counterpart of these constraints while introducing the fractions of presence of each phase, namely the volume fraction $\alpha_k = V_k/V \in [0, 1]$, the mass fraction $y_k = M_k/M \in [0, 1]$ and the entropy fraction $z_k = S_k/S \in [0, 1]$, such that

(18)
$$y_k \tau_k = \alpha_k \tau, \quad y_k s_k = z_k s.$$

Then the intensive counterpart of the extensive constraints reads

(19)
$$\begin{cases} 1 = \alpha_1 + \alpha_2, \\ 1 = y_1 + y_2, \\ 1 = z_1 + z_2 + z_i, \end{cases}$$

where $z_i = S_i/S \in [0, 1]$ stands for the entropy fraction of the interface.

We now turn to the definition of the extensive energy of the whole system. It corresponds to the sum of the energies of each part, namely

(20)
$$E(M, V, S, A_i) = E_1(M_1, V_1, S_1) + E_2(M_2, V_2, S_2) + E_i(S_i, A_i).$$

Using the fractions definitions, the total derivative of E reads

$$dE = \sum_{k=1}^{2} (T_k dS_k - p_k dV_k + \mu_k dM_k) + T_i dS_i + \gamma_i dA_i$$
$$= \sum_{k=1}^{2} (T_k z_k dS + ST_k dz_k - p_k \alpha_k dV_k - V p_k d\alpha_k$$
$$+ y_k \mu_k dM_k + M \mu_k dy_k)$$
$$+ T_i z_i dS + ST_i dz_i + \gamma_i a_i dV + \gamma_i V da_i.$$

Reorganizing the terms and using the intensive constraints (19), one obtains

Proposition 1. The extensive energy satisfies

(21)

$$dE = (z_1T_1 + z_2T_2 + z_iT_i)dS - (\alpha_1p_1 + \alpha_2p_2 - a_i\gamma_i)dV + y_1(\mu_1 - \mu_2)dM + S((T_1 - T_i)dz_1 + (T_2 - T_i)dz_2) - V((p_1 - p_2)d\alpha_1 - \gamma_ida_i) + M(\mu_1 - \mu_2)dy_1.$$

As a consequence, the temperature, pressure and chemical potential of the fluidinterface system have natural definitions in terms of the phasic and interfacial quantities:

(22)
$$\begin{cases} T := z_1 T_1 + z_2 T_2 + z_i T_i, \\ p := \alpha_1 p_1 + \alpha_2 p_2 - a_i \gamma_i, \\ \mu := y_1 \mu_1 + y_2 \mu_2. \end{cases}$$

In absence of the surface tension, the mixture pressure coincides with the mixture pressure classic bi-fluid or two-phase models [25]. When accounting for surface tension, the mixture pressure is exactly the one of the two-phase flow model, derived in [23] by homogenization techniques. This pressure also appears in jump conditions of Euler-Korteweg system, see [24]. The pressure we get is also close to the pressure term derived in [8, 7] in the context of two-phase flows with surface tension.

For a given state (M, V, E, A_i) , and according to the second principle of thermodynamics, the thermodynamical equilibrium corresponds to a minimum of the energy E defined in (20) under the extensive constraints (15)-(17). Thus, in the interior of the constraint set, the derivatives of E with respect to independent variables cancel, leading to a characterization of the thermodynamical equilibrium in terms of phasic potentials.

Proposition 2. According to the differential form (21), the thermodynamical equilibrium is characterized by

(23)
$$\begin{cases} \mu_1 = \mu_2, \\ T_1 = T_2 = T_i, \\ \gamma_i da_i - (p_1 - p_2) d\alpha_1 = 0. \end{cases}$$

The two first equalities of (23) are classic: they denote the thermal equilibrium in the fluid-interface system and the mass transfer between the two fluid phases. The last (differential) relation represents the mechanical equilibrium, and brings out some comments:

- As $\gamma_i = 0$, that is for a planar interface, one recovers that the mechanical equilibrium corresponds to the saturation of the phasic pressures $p_1 = p_2$ (see for instance [5]);
- Assume that the phase 1 occupies a spherical bubble of radius R. Then its volume is $V_1 = 4\pi R^3/3$ and the interfacial area is $A_i = 4\pi R^2$. On the other hand the differential relation in (23) gives

$$\gamma d\left(\frac{A_{i}}{V}\right) - (p_{1} - p_{2})d\left(\frac{V_{1}}{V}\right) = 0$$

Expressing this latter formula in terms of the radius R, it leads to the Young-Laplace law

$$p_1 - p_2 = \frac{2\gamma_i}{R}.$$

Classically the Young-Laplace law involves the mean curvature which corresponds here to the inverse of the radius. When the radius tends to $+\infty$, the surface becomes planar and one recovers the equality of the phasic pressures.

2.4. Another characterization of the thermodynamical equilibrium using free energies. In the context of two-phase flows in porous media, Smaï proposed in [32] to minimize the free energy of the mixture instead of minimizing the energy. The advantage is that the free energy of the mixture (also called canonical grand potential in the porous media framework) is solely a function of the mixture temperature and the phasic pressures.

In the extensive framework, the free energy Ω_k of the phase k = 1, 2 is defined as the (total) Legendre transform of the energy E_k :

(24)
$$\Omega_k = E_k - T_k S_k - \mu_k M_k$$

Differentiating (24) and using the Gibbs relation (1) give

(25)
$$d\Omega_k = -p_k dV_k - S_k dT_k - M_k d\mu_k.$$

In order to introduce intensive potential, it is convenient to scale with respect to the volume V_k to define the intensive (volumic) free energy $\omega_k = \Omega_k/V_k$. Then using the definitions (18), it holds

$$\alpha_k \omega_k = \frac{e_k}{\tau_k} \alpha_k - T_k \frac{s_k}{\tau_k} \alpha_k - \frac{\mu_k}{\tau_k} \alpha_k,$$

from which one deduces the following differential form

(26)
$$d(\alpha_k \omega_k) = -p_k d\alpha_k - \frac{\alpha_k s_k}{\tau_k} dT_k - \frac{\alpha_k}{\tau_k} d\mu_k,$$

using the intensive relations (5) and (6).

As the interfacial potentials are concerned, the free energy is defined as a partial Legendre transform of the energy E_i , namely

(27)
$$\Omega_{\rm i} = E_{\rm i} - T_{\rm i} S_{\rm i}.$$

Using the interfacial Gibbs relation (7), it yields

(28)
$$d\Omega_{i} = -S_{i}dT_{i} + \gamma_{i}dA_{i}.$$

The appropriate intensive free energy is deduced by scaling with respect to the interfacial area: $\omega_i = \Omega_i / A_i$. Hence the intensive free energy reads

(29)
$$a_{i}\omega_{i} = a_{i}e_{i} - T_{i}a_{i}s_{i}$$

whose differential is

(30) $d(a_i\omega_i) = a_is_i dT_i + \gamma_i da_i,$

according to (13).

For the fluid-interface system, the extensive free energy corresponds to the sum of the phasic and interfacial free energies

$$\Omega = \Omega_1 + \Omega_2 + \Omega_i,$$

whose intensive formulation is

(31)
$$\omega = \alpha_1 \omega_1 + \alpha_2 \omega_2 + a_i \omega_i.$$

According to the differentials (26) and (30), it yields

(32)
$$d\omega = -(p_1 - p_2)\mathrm{d}\alpha_1 + \gamma_i\mathrm{d}a_i - \alpha_1\mathrm{d}p_1 - \alpha_2\mathrm{d}p_2 + a_is_i\mathrm{d}T_i,$$

since $\alpha_1 + \alpha_2 = 1$.

At thermodynamical equilibrium, the phasic and interfacial potentials agree with (23). As a consequence the thermodynamical equilibrium has to comply with an equation of state compatible with

(33)
$$d\omega = -\alpha_1 \mathrm{d}p_1 - \alpha_2 \mathrm{d}p_2 + as_i \mathrm{d}T.$$

This differential implies that the equation of state of the fluid-interface system can be expressed in term ω , seen as a function of T and p_k , k = 1, 2, such that

$$as_{i} = \frac{\partial \omega}{\partial T}(T, p_{1}, p_{2}), \quad \alpha_{k} = -\frac{\partial \omega}{\partial p_{k}}(T, p_{1}, p_{2}).$$

The idea of Smaï is to take advantage of this alternative description of the thermodynamical equilibrium to get rid of the complex description of the interface: from the equation of state $\omega(T, p_1, p_2)$, one recovers all the information relative to the interface, without explicitly computing the interfacial area.

This approach is not developed here since we precisely want to derive an evolution equation of the interfacial area.

2.4.1. Potential energy candidate. We can now turn to the definition of the potential energy which will be used in the Lagrangian formulation. A natural proposition would be to consider the intensive mixture internal energy when scaling the extensive energy (20) by the total mass M. Then for a given intensive state (τ, s, a_i) , accounting for the intensive constraints (19), the intensive energy would read

(34)
$$e(\tau, s, a_{i}, (y_{k})_{k}, (\alpha_{k})_{k}, (z_{k})_{k}, z_{i}) = y_{1}e_{1}(\tau_{1}, s_{1}) + y_{2}(\tau_{2}, s_{2}) + a_{i}\tau e_{i}\left(\frac{z_{i}}{a}\frac{s}{\tau}\right),$$

with notations (18) of the phasic quantities.

However it turns out that this choice of variables is not appropriate. Indeed it is not clear how the entropy fractions z_k evolve along trajectories when applying the Stationary Action Principle whereas specific entropies are conserved along trajectories, according to [20, 16]. Hence it is more convenient to express the intensive fluid-interface internal energy as a function of the intensive entropies s and s_k , k = 1, 2 rather than using the entropy fractions z_k .

In the sequel, we choose to express the intensive energy as a function of

(35)
$$\mathbf{B} = \{\rho, s, s_1, s_2, a_i, y, \alpha\},\$$

where $\rho = 1/\tau$ denotes the mixture density and $y := y_1$ and $\alpha := \alpha_1$. It reads then

(36)
$$e(\tilde{\mathbf{B}}) = ye_1\left(\frac{\alpha}{y\rho}, s_1\right) + (1-y)e_2\left(\frac{1-\alpha}{(1-y)\rho}, s_2\right) + \frac{a_i}{\rho}e_i\left(\frac{s-ys_1-(1-y)s_2}{a_i}\rho\right).$$

Observe that one makes use of the extensive relation (17) on the entropies to express the interfacial entropy s_i as a function of s, s_1 and s_2 , namely

(37)
$$s = ys_1 + (1-y)s_2 + \frac{a_i}{\rho}s_i.$$

Remark 1. In [6, paragraph 2.1.3.3], the author points out the importance of the choice of variables on which the Lagrangian functional depends. This is also emphasized in the work of Gavrilyuk [15]. Indeed if specific entropies are convenient variables for computations, the fact that they are conserved along trajectories prohibits any interaction between the phases. The fluid-interface entropy will also be conserved since only reversible processes can be depicted by the SAP. However it is possible to add relaxation source terms a posteriori, in agreement with the second law of thermodynamics. See [9, Paragraph 3.5] for a presentation of the method when dissipation is due to pulsating behaviour of bubbles in two-phase flows.

3. Derivation of the evolution equations by means of Stationary Action Principle

Accounting for the previous characterization of the thermodynamical equilibrium, we now turn to the modelling of the fluid dynamics. The objective is to derive the Euler-type equations satisfied by the fluid-interface system using the Stationary Action Principle, following the serie of works [20, 17, 10, 8, 7, 9, 30].

We focus on homogeneous two-phase flows, in the sense that the two phases evolve with the same velocity field $\mathbf{u} \in \mathbb{R}^3$. Note that considering distinct velocities is possible as in [17].

The variational approach and the Hamilton's principle of stationary action rely on the definition of an appropriate Lagrangian L. This Lagrangian is the difference

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of a kinetic energy and a potential energy. The potential energy we propose to consider has been derived in the previous section, see (36). As far as the kinetic one is concerned, a small review of recent models is given in Section 3.1, focusing on the so-called *two-scale kinetic* modelling brought forward in [10, 6].

In Section 3.2 are stated the main lines of the SAP as well as the additional assumptions we make (total and partial mass conservations for instance). As a result is presented the final set of equations, in its rough form.

3.1. A non-exhaustive review of kinetic energy. Recent references takle the derivation of the kinetic energy, motivated by the initial works of Gavrilyuk and coauthors [20, 17]. In the latter propositions, the kinetic energy L_{kin} is composed of a classic bulk energy linked to the translational motion of the fluid and a small scale contribution T_{pulse} . For instance in [17], considering distinct velocities for both the phases k = 1, 2 and the interface, it yields

$$L_{kin} = \sum_{k=1}^{2} \rho_k \frac{|\mathbf{u}_k|^2}{2} + T_{pulse},$$

where \mathbf{u}_k stands for the velocity field of the phase k and

$$T_{pulse} = \frac{m}{2} \left(\frac{\mathrm{D}_{\mathrm{i}} \alpha}{\mathrm{D} t} \right)^2,$$

where $\frac{\mathbf{D}_{\mathbf{i}}}{\mathbf{D}t}$ is the material derivative associated to the velocity of the interface $\mathbf{u}_{\mathbf{i}}$, namely $\frac{\mathbf{D}_{\mathbf{i}}}{\mathbf{D}t} = \partial_t \cdot + \mathbf{u}_{\mathbf{i}} \cdot \nabla_{\mathbf{x}} \cdot$.

According to the authors, the second term is a pulsation kinetic energy, where the coefficient m and the interfacial velocity \mathbf{u}_i are given by appropriate closure laws. Considering a one-velocity model, Drui proposes in [10] to consider $T_{pulse} = \frac{1}{2}\nu(\alpha)|\mathbf{D}_t\alpha|^2$. The function ν corresponds to the inertia associated with the motion of the interface which depends on the volume fraction α only. Another improvement is introduced by Cordesse [6, 8], where the function ν is a function of the interfacial area, namely $T_{pulse} = \frac{1}{2}m\frac{|\mathbf{D}_t\alpha|^2}{a_i^2}$. Here and in the sequel, the material derivative is defined using the common velocity field \mathbf{u}

$$\mathbf{D}_t \cdot = \partial_t \cdot + \mathbf{u} \cdot \nabla_{\mathbf{x}} \cdot .$$

This last expression of T_{pulse} is derived from geometrical considerations: when the interface is subjected to a small displacement, the interfacial area a_i and the volume fraction α vary as well, and the relationships between these quantities involve the local curvature of the interface and the surface tension parameter, see [6, Chapter 3] for more details. Finally in [9] the function ν is no longer an explicit function of α or a_i . The pulsating energy reads

$$T_{pulse} = \frac{1}{2}\nu(\alpha, a_{\rm i})|\mathbf{D}_t h|^2,$$

where h is the local deformation of the interface, which satisfies differential relations involving the interfacial area, the local curvature and the volume fraction.

Among all the propositions, what is mandatory is to make the kinetic energy L_{kin} depends on $D_t \alpha$, otherwise there will we be no hope to get an evolution equation on

 α . For the same reason and because we want an evolution equation of the interfacial area density, we propose to consider also a term involving $D_t a_i$:

(38)
$$L_{kin} = \frac{1}{2}\rho |\mathbf{u}|^2 + \frac{m}{2}|\mathbf{D}_t\alpha|^2 + \frac{\nu}{2}|\mathbf{D}_ta_i|^2,$$

where m and ν are constants (with the appropriate dimensions, namely $m[kg \cdot m^{-1}]$ and $\nu[kg \cdot m]$). Doing so ensures to get an evolution equation of the interfacial area density, without considering any additional quantities as local curvature or interface displacement as in [6, 8].

3.2. The Lagrangian functional and additional assumptions. We introduce the vector of variables **B**

(39)
$$\mathbf{B} := \{\rho, s, s_1, s_2, a_i, y, \alpha, \mathbf{u}, \mathbf{D}_t \alpha, \mathbf{D}_t a_i\}$$

which corresponds to the vector $\tilde{\mathbf{B}}$, defined in (35), completed by the variables involved in the kinetic energy L_{kin} , that are \mathbf{u} , $D_t \alpha$ and $D_t a_i$.

The Lagrangian L, function of **B**, is the difference of the kinetic and the potential contribution

(40)
$$L(\mathbf{B}) = L_{kin} - L_{pot},$$

where $L_{kin}(\mathbf{B})$ is defined in (38) and $L_{pot}(\mathbf{B}) = \rho e(\tilde{\mathbf{B}})$, with $e(\tilde{\mathbf{B}})$ defined in (36).

Before going further with the variational method, we make additional assumptions that govern the fluid-interface system. First we assume masses conservation, in the sense that

(41)
$$\begin{aligned} \partial_t \rho + \operatorname{div}_{\mathbf{x}}(\rho \mathbf{u}) &= 0, \\ \mathbf{D}_t y &= 0. \end{aligned}$$

One emphasizes that although the modelling presented in Section 2.3 allows mass exchange between the two phases, it is not the case here. This is due to the fact that SAP is valid for reversible processes only. For the same reasons, we also assume that the specific entropies are conserved along trajectories

(42)
$$D_t s = 0, \quad D_t s_k = 0, \quad k = 1, 2,$$

following [20, 17, 6]. Notice that, since the specific phasic entropies are conserved, the interface intensive entropy (which is relative to the interfacial area A_i and not to mass M) is not conserved along trajectories but satisfies

$$\mathbf{D}_t(s_{\mathbf{i}}a_{\mathbf{i}}\tau) = 0$$

that is to say, using extensive variables, $s_i a_i \tau = S_i / M$ is constant along trajectories.

3.3. Variational principle. This paragraph recalls the classic lines of the Stationary Action Principle, whose application to the two-phase flow modeling has been the subjects of numerous works, including [11, 2, 18, 19, 4]. See also [9] for a synthetic presentation of the method and an overview of the technic in the two-fluid framework.

Consider a volume $\omega(t) \in \mathbb{R}^3$ occupied by the fluid-interface system for time $t \in [t_1, t_2]$ and denote $\Omega = \{(t, \mathbf{x}) \in \times [t_1, t_2] \times \mathbb{R}^d | \mathbf{x} \in \omega(t), t_1 \leq t \leq t_2\}$. Following Section 3.2, we assume the flow to be fully characterized by the quantities $(t, \mathbf{x}) \mapsto \mathbf{B}$

and by the constitutive constraints (41)-(42). We now define the Hamiltonian Action as the space-time integral of the Lagrangian functional (40)

(43)
$$A(\mathbf{B}) = \int_{\Omega} L(\mathbf{B})(\mathbf{x}, t) \mathrm{d}\mathbf{x} \mathrm{d}t,$$

and apply the Stationary Action principle. If $(t, \mathbf{x}) \mapsto \mathbf{\bar{B}}$ is a physically relevant transformation of the system, it is the solution of a variational problem leading to a PDE system. The methodology is to consider a family of perturbation $(t, \mathbf{x}, \zeta) \mapsto \mathbf{B}_{\zeta}$ of $\mathbf{\bar{B}}$, parametrized by $\zeta \in [0, 1]$ such that

• the physical path is obtained when $\zeta = 0$:

$$\mathbf{B}_{\zeta}(t, \mathbf{x}, \zeta = 0) = \bar{\mathbf{B}}(t, \mathbf{x}),$$

- \mathbf{B}_{ζ} satisfies the conservation constraints (41) and (42) for all $\zeta \in [0, 1]$,
- $\mathbf{B}_{\zeta}(t, \mathbf{x}, \zeta) = \overline{\mathbf{B}}(t, \mathbf{x})$ for $(t, \mathbf{x}, \zeta) \in \partial \Omega \times [0, 1]$.

The Stationary Action Principle states that $\overline{\mathbf{B}}$ is physically relevant if it is a stationary point of $\zeta \mapsto A(\mathbf{B}_{\zeta})$, that is

(44)
$$\frac{\mathrm{d}A(\mathbf{B}_{\zeta})}{\mathrm{d}\zeta}(0) = 0.$$

This stationary condition yields the governing set of PDEs of motion without dissipative process. For $b \in \overline{\mathbf{B}}$, denoting

$$\delta_{\zeta} b(t, \mathbf{x}) = \left(\frac{\partial b_{\zeta}}{\partial \zeta}\right)_{|t, \mathbf{x}} (t, \mathbf{x}, \zeta = 0)$$

a family of infinitesimal transformations, the identity (44) reads

(45)
$$\frac{\mathrm{d}A(\mathbf{B}_{\zeta})}{\mathrm{d}\zeta}(\zeta=0) = \int_{\Omega} \sum_{b\in\mathbf{B}} \frac{\partial L}{\partial b} \delta_{\zeta} b \mathrm{d}\mathbf{x} \mathrm{d}t.$$

Infinitesimal variations are related through the conservation principles (41) and (42) (see [14] and [4] for detailed computations)

• variation of density

(46)
$$\delta \rho = -\operatorname{div}_{\mathbf{x}}(\rho \delta \mathbf{x})$$

where $\delta \mathbf{x}$ denotes the infinitesimal displacement $(t, \mathbf{x}) \mapsto \delta \mathbf{x}$ around the physical path, which complies with $\delta \mathbf{x}_{|t=t_1} = \delta \mathbf{x}_{|t=t_2} = 0$ and $\delta \mathbf{x}_{|\partial \omega(t)} = 0$. • variation of velocity

(47)
$$\delta \mathbf{u} = \mathbf{D}_t(\delta \mathbf{x}) - \nabla_{\mathbf{x}} \mathbf{u} \cdot \delta \mathbf{x},$$

• conservation along trajectories of the fluid specific entropies and the mass fraction

(48)
$$\delta b = -\nabla_{\mathbf{x}} b \cdot \delta \mathbf{x}, \quad \text{for } b \in \{s, y, z_1, z_2\}.$$

We now list all the contributions in (45).

• Density contribution: using the mass conservation (41), one has

(49)
$$\int_{\Omega} \frac{\partial L}{\partial \rho} \delta \rho \mathrm{d}\mathbf{x} \mathrm{d}t = -\int_{\Omega} \frac{\partial L}{\partial \rho} \mathrm{div}_{\mathbf{x}}(\rho \delta \mathbf{x}) \, \mathrm{d}\mathbf{x} \mathrm{d}t$$
$$= \int_{\Omega} \rho \nabla_{\mathbf{x}} \left(\frac{\partial L}{\partial \rho}\right) \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t,$$

by integration by parts. In order to make the partial Legendre transform of L with respect to ρ (written here as a function of **B**)

(50)
$$L^{*,\rho}(\mathbf{B}) = \rho \frac{\partial L}{\partial \rho} - L(\mathbf{B})$$

appear, one develops

(51)

$$\int_{\Omega} \frac{\partial L}{\partial \rho} \delta \rho \, \mathrm{d}\mathbf{x} \mathrm{d}t$$

$$= \int_{\Omega} \left[\nabla_{\mathbf{x}} \left(\rho \frac{\partial L}{\partial \rho} \right) - \frac{\partial L}{\partial \rho} \nabla_{\mathbf{x}} \rho \right] \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t$$

$$= \int_{\Omega} \left[\nabla_{\mathbf{x}} \left(\rho \frac{\partial L}{\partial \rho} - L \right) + \nabla_{\mathbf{x}} L - \frac{\partial L}{\partial \rho} \nabla_{\mathbf{x}} \rho \right] \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t$$

$$= \int_{\Omega} \left(\nabla_{\mathbf{x}} L^{*,\rho} + \sum_{\substack{b \in \mathbf{B} \\ b \neq \rho}} \nabla_{\mathbf{x}} b \frac{\partial L}{\partial b} \right) \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t.$$

• Velocity contribution: according to (47), it holds

(52)
$$\int_{\Omega} \frac{\partial L}{\partial \mathbf{u}} \delta \mathbf{u} \, \mathrm{d}\mathbf{x} \mathrm{d}t = \int_{\Omega} \frac{\partial L}{\partial \mathbf{u}} \left(\mathrm{D}_t(\delta \mathbf{x}) - \nabla_{\mathbf{x}} \mathbf{u} \cdot \delta \mathbf{x} \right) \mathrm{d}\mathbf{x} \mathrm{d}t.$$

By definition of the material derivative $\mathbf{D}_t\cdot$ and using an integration by part, it holds

(53)
$$\int_{\Omega} \frac{\partial L}{\partial \mathbf{u}} \delta \mathbf{u} \, \mathrm{d} \mathbf{x} \mathrm{d} t$$
$$= \int_{\Omega} \frac{\partial L}{\partial \mathbf{u}} \left[\partial_t (\delta \mathbf{x}) + \mathbf{u} \cdot \nabla_{\mathbf{x}} (\delta \mathbf{x}) - \nabla_{\mathbf{x}} \mathbf{u} \cdot \delta \mathbf{x} \right] \mathrm{d} \mathbf{x} \mathrm{d} t$$
$$= -\int_{\Omega} \left(\partial_t \left(\frac{\partial L}{\partial \mathbf{u}} \right) + \mathrm{div}_{\mathbf{x}} \left(\mathbf{u} \frac{\partial L}{\partial \mathbf{u}} \right) + \frac{\partial L}{\partial \mathbf{u}} \nabla_{\mathbf{x}} \mathbf{u} \right) \cdot \delta \mathbf{x} \, \mathrm{d} \mathbf{x} \mathrm{d} t.$$

• Contributions of conserved quantities along trajectories: using (48), it holds for $b \in \{s, s_1, s_2, y\}$

(54)
$$\int_{\Omega} \frac{\partial L}{\partial b} \delta b \, \mathrm{d}\mathbf{x} \mathrm{d}t = -\int_{\Omega} \frac{\partial L}{\partial b} \nabla_{\mathbf{x}} b \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t.$$

- Contributions in α and a_i : the variation of the volume fraction α is not subjected to any constraint. Doing so ensures to get an evolution equation on α . Therefore the variation $\delta \alpha$, involved with the family of transformations of the medium, is arbitrary. The same holds for the interfacial area density a_i . Besides, the fact that they evolve independently will yield separate equations for the volume fraction and the interfacial area density.
- Contributions in $D_t \alpha$ and $D_t a_i$: the variations of $D_t \alpha$ (resp. $D_t a_i$) is related to the variation of α (resp. a_i). According to [26], it holds, for any functions f and g, it holds

(55)
$$\int_{\Omega} g \,\delta(\mathbf{D}_t f) \,\mathrm{d}\mathbf{x} \mathrm{d}t = -\int_{\Omega} \left(\partial_t g + \mathrm{div}_{\mathbf{x}}(\mathbf{u}g)\right) \delta f \,\mathrm{d}\mathbf{x} \mathrm{d}t \\ -\int_{\Omega} \left[(\partial_t g + \mathrm{div}_{\mathbf{x}}(\mathbf{u}g)) \nabla_{\mathbf{x}} f + g \nabla_{\mathbf{x}}(D_t f) \right] \cdot \delta \mathbf{x} \,\mathrm{d}\mathbf{x} \mathrm{d}t.$$

Thus using (55) with $g = \frac{\partial L}{\partial(\mathbf{D}_t \alpha)} =: M$ and $f = \mathbf{D}_t \alpha$ gives

(56)
$$\int_{\Omega} \frac{\partial L}{\partial(\mathbf{D}_{t}\alpha)} \delta(\mathbf{D}_{t}\alpha) \, \mathrm{d}\mathbf{x} \mathrm{d}t$$
$$= -\int_{\Omega} (\partial_{t}M + \operatorname{div}_{\mathbf{x}}(M\mathbf{u})) \delta\alpha \, \mathrm{d}\mathbf{x} \mathrm{d}t$$
$$-\int_{\Omega} ((\partial_{t}M + \operatorname{div}_{\mathbf{x}}(M\mathbf{u})) \nabla_{\mathbf{x}}\alpha + M \nabla_{\mathbf{x}}(\mathbf{D}_{t}\alpha)) \cdot \delta\mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t.$$

Analogously it holds with $g = \frac{\partial L}{\partial (\mathbf{D}_t a_\mathbf{i})} =: P$ and $f = \mathbf{D}_t a_\mathbf{i}$

(57)
$$\int_{\Omega} \frac{\partial L}{\partial (\mathbf{D}_{t} a_{i})} \delta(\mathbf{D}_{t} a_{i}) \, \mathrm{d}\mathbf{x} \mathrm{d}t$$
$$= -\int_{\Omega} (\partial_{t} P + \operatorname{div}_{\mathbf{x}}(P\mathbf{u})) \delta a_{i} \, \mathrm{d}\mathbf{x} \mathrm{d}t$$
$$-\int_{\Omega} ((\partial_{t} P + \operatorname{div}_{\mathbf{x}}(P\mathbf{u})) \nabla_{\mathbf{x}} a_{i} + P \nabla_{\mathbf{x}}(\mathbf{D}_{t} a_{i})) \cdot \delta \mathbf{x} \, \mathrm{d}\mathbf{x} \mathrm{d}t.$$

Finally gathering (51), (53), (56) and (57) gives

$$\int_{\Omega(0)} [A_{\alpha} \delta \alpha + A_{a_{i}} \delta a_{i} + A_{\mathbf{u}} \delta \mathbf{x}] \, \mathrm{d}\mathbf{x} \mathrm{d}t = 0.$$

where

(58)
$$\begin{cases} A_{\alpha} = \partial_t M + \operatorname{div}(M\mathbf{u}) - \frac{\partial L}{\partial \alpha}, & \text{with } M = \frac{\partial L}{\partial(\mathbf{D}_t \alpha)}, \\ A_{a_i} = \partial_t P + \operatorname{div}(P\mathbf{u}) - \frac{\partial L}{\partial a_i}, & \text{with } P = \frac{\partial L}{\partial(\mathbf{D}_t a_i)}, \\ A_{\mathbf{u}} = \partial_t K + \operatorname{div}(K\mathbf{u}) - \nabla L^{*,\rho}, & \text{with } K = \frac{\partial L}{\partial \mathbf{u}}. \end{cases}$$

Note that to express the term C, one makes use of the terms A and B.

Since one assumes the infinitesimal displacement and the variations of volume fraction and interfacial area density to be independent, the SAP applied to the Lagrangian energy L yields the equations of motion given by

$$A_{\alpha} = 0, \quad A_{a_{\mathbf{i}}} = 0, \quad A_{\mathbf{u}} = 0.$$

4. Final system and properties

As a result of the Stationary Action Principle, one obtains the following set of equations describing the time evolution of the fluid-interface system governed by the Lagrangian L. It reads

(59)
$$\begin{cases} \partial_t M + \operatorname{div}(M\mathbf{u}) - \frac{\partial L}{\partial \alpha} = 0, \\ \partial_t P + \operatorname{div}(P\mathbf{u}) - \frac{\partial L}{\partial a_i} = 0, \\ \partial_t K + \operatorname{div}(K\mathbf{u}) - \nabla L^{*,\rho} = 0, \end{cases}$$

where $L^{*,\rho}$ the partial Legendre transform of L defined in (50), and it is completed by the mass conservation laws (41) and the entropies evolution equations (42).

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Actually the SAP ensures conservation principle (as a consequence of the Noether's theorem, see [4]). Let \mathcal{E} be the partial Legendre transform of the Lagrangian L with respect to the *kinetic* variables \mathbf{u} , $D_t \alpha$ and $D_t a_i$. It reads

(60)
$$\mathcal{E}(\rho, K, M, P, \alpha, a_{i}, s, s_{1}, s_{2}, y) = \mathbf{u}K + \mathbf{D}_{t}\alpha M + \mathbf{D}_{t}a_{i}P - L(\mathbf{B})$$

or analogously

(61)
$$\mathcal{E}(\mathbf{B}) = L_{kin}(\mathbf{B}) + L_{pot}(\mathbf{B}),$$

with notations (40). If the latter formula is more classic, the definition (60) has the advantage of simplifying the following computations.

Proposition 3 (Hyperbolicity). The energy \mathcal{E} , defined by (60), satisfies the additional scalar conservation equation

(62)
$$\partial_t \mathcal{E} + div((\mathcal{E} - L^{*,\rho})\mathbf{u}) = 0.$$

If the energy $\mathcal{E}(\rho, K, M, P, \alpha, a_i, s, s_1, s_2, y)$ is convex, then the system (41)-(42)-(59) is hyperbolic and it is symmetrizable.

Proof. Using that \mathcal{E} is the partial Legendre transform of the Lagrangian L with respect to the kinetic variables, it holds (dropping the dependency of \mathcal{E} and L for readability)

$$D_{t}\mathcal{E} = D_{t}\left(\sum_{b \in \{\mathbf{u}, D_{t}\alpha, D_{t}a_{i}\}} b\frac{\partial L}{\partial b} - L\right)$$
$$= \sum_{b \in \{\mathbf{u}, D_{t}\alpha, D_{t}a_{i}\}} \left(D_{t}b\frac{\partial L}{\partial b} + bD_{t}\left(\frac{\partial L}{\partial b}\right)\right) - D_{t}L$$

Using the notations K, M and P, given in (58), and the transport of the specific entropies (42) and of the mass fraction (41), it holds

$$\mathbf{D}_t \mathcal{E} = \mathbf{u} \mathbf{D}_t K + \mathbf{D}_t \alpha \mathbf{D}_t M + \mathbf{D}_t a_i \mathbf{D}_t P - \frac{\partial L}{\partial \rho} \mathbf{D}_t \rho - \frac{\partial L}{\partial \alpha} \mathbf{D}_t \alpha - \frac{\partial L}{\partial a_i} \mathbf{D}_t a_i.$$

Then using the evolution equations (59), it yields

$$D_{t}\mathcal{E} = \mathbf{u} \cdot \left(-K \operatorname{div}_{\mathbf{x}}(\mathbf{u}) + \nabla_{\mathbf{x}} L^{*,\rho}\right) + D_{t}\alpha \left(-M \operatorname{div}_{\mathbf{x}}(\mathbf{u}) + \frac{\partial L}{\partial \alpha}\right) + D_{t}a_{i}\left(-P \operatorname{div}_{\mathbf{x}}(\mathbf{u}) + \frac{\partial L}{\partial a_{i}}\right) - \frac{\partial L}{\partial \rho}D_{t}\rho - \frac{\partial L}{\partial \alpha}D_{t}\alpha - \frac{\partial L}{\partial a_{i}}D_{t}a_{i} = -\operatorname{div}_{\mathbf{x}}(\mathbf{u})\left(K\mathbf{u} + MD_{t}\alpha + PD_{t}a_{i} - \rho\frac{\partial L}{\partial \rho}\right) + \mathbf{u} \cdot \nabla_{\mathbf{x}}\left(\rho\frac{\partial L}{\partial \rho} - L\right)$$

Using the definition (60) of \mathcal{E} , it gives

$$D_t \mathcal{E} = -\text{div}_{\mathbf{x}}(\mathbf{u}) \left(\mathcal{E} + L - \rho \frac{\partial L}{\partial \rho} \right) + \mathbf{u} \cdot \nabla_{\mathbf{x}} L^{*,\rho}$$
$$= -\text{div}_{\mathbf{x}}(\mathbf{u}) \left(\mathcal{E} - \nabla_{\mathbf{x}} L^{*,\rho} \right) + \mathbf{u} \cdot \nabla_{\mathbf{x}} L^{*,\rho},$$

which coincides with (62). Now if \mathcal{E} is supposed to be convex with respect to the variables $(\rho, K, M, P, \alpha, a_i, s, s_1, s_2, y)$, then it is a Lax entropy of the system which can be symmetrized in the sense of Godunov-Mock.

Note that the sufficient criterion is quite restrictive since the potential energy $L_{pot}(\mathbf{B}) = \rho e(\tilde{\mathbf{B}})$ is not necessarily strictly convex.

4.1. Extended final set. We explicit in this paragraph the three equations using the definition (40) of the Lagrangian functional.

4.1.1. Momentum equation. By the definition (50), the Legendre transform of L with respect to the density $L^{*,\rho}$ is

(63)
$$L^{*,\rho}(\mathbf{B}) = -\left(\frac{m}{2}|\mathbf{D}_t\alpha|^2 + \frac{\nu}{2}|\mathbf{D}_ta_i|^2 + p\right),$$

with

(64)
$$p = \alpha p_1 + (1 - \alpha) p_2 - a_i \gamma_i,$$

momentum equation, namely

is the fluid-interface pressure derived first in (22). Here one uses $p_1 := p_1\left(\frac{\alpha}{y\rho}, s_1\right)$ and $p_2 := p_2\left(\frac{1-\alpha}{(1-y)\rho}, s_2\right)$. Then the equation on $K = \partial L/\partial \mathbf{u} = \rho \mathbf{u}$ gives the

$$\partial_t(\rho \mathbf{u}) + \operatorname{div}_{\mathbf{x}}(\rho \mathbf{u}^\top \mathbf{u}) + \nabla_{\mathbf{x}} \left(p + \frac{m}{2} |D_t \alpha|^2 + \frac{\nu}{2} |D_t a_i|^2 \right) = 0.$$

This equation is similar to the one obtained in [10] or [8], except that, in this latter reference, the pressure term accounts for $\nabla_{\mathbf{x}} \alpha$. When dropping the small scale terms $D_t \alpha$ and $D_t a_i$, one recovers the momentum flux derived in [23] for bubbly flows using an homogenization approach. The pressure term p comes from the potential energy L_{pot} which defines the pressure term in the momentum equation.

4.1.2. Evolution equations on α and a_i . Since $M = mD_t\alpha$ and $P = \nu D_t a_i$, the equations on M and P involve second order derivatives in time on α and a_i respectively. Using the definition (40) of L, and relations (11)-(12), direct computations give

(65)
$$\frac{\partial L}{\partial \alpha} = p_1 - p_2, \qquad \frac{\partial L}{\partial a_i} = \gamma_i,$$

which lead to

(66)
$$\begin{cases} \partial_t(\mathbf{D}_t\alpha) + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\mathbf{D}_t\alpha) = \frac{p_1 - p_2}{m} \\ \partial_t(\mathbf{D}_ta_i) + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\mathbf{D}_ta_i) = \frac{\gamma_i}{\nu}. \end{cases}$$

Following [10, 8], the idea is to decompose these second order equations into a pair of two first order derivative in time equations, while introducing additional unknowns.

For the equation on $M = m D_t \alpha$, we fix

(67)
$$\mathbf{D}_t \alpha = \frac{\rho y w}{\sqrt{m}},$$

where w is a new unknown. Then it holds

(68)
$$\begin{cases} \partial_t \alpha + \mathbf{u} \cdot \nabla_{\mathbf{x}} \alpha = \frac{pgw}{\sqrt{m}}, \\ \partial_t w + \mathbf{u} \cdot \nabla_{\mathbf{x}} w = \frac{1}{\sqrt{m}\rho y} (p_2 - p_1) \end{cases}$$

Doing so for the equation on $P = \nu D_t a_i$, we introduce the unknown *n* satisfying

(69)
$$D_t a_i = \frac{\rho g n}{\sqrt{\nu}},$$

and it yields

(70)
$$\begin{cases} \partial_t a_{\mathbf{i}} + \mathbf{u} \cdot \nabla_{\mathbf{x}} a_{\mathbf{i}} = \frac{\rho y n}{\sqrt{\nu}}, \\ \partial_t n + \mathbf{u} \cdot \nabla_{\mathbf{x}} n = \frac{\gamma_i}{\sqrt{\nu} \rho y} \end{cases}$$

According to [8, 6, 9], the equations on the quantities w and n, defined in this way, refer to small scale momentum equations. In that sense the equations on α and a_i connect small and large scales.

4.1.3. *Energy equations.* The transport equations of the specific entropies are not convenient, especially for numerical computations. We replace them by energy equations using the Gibbs relations given in Section 2.

The total energy equation $\mathcal{E} = L_{kin} + L_{pot}$ has already been given in (62), see Proposition 3, and its developed form reads

(71)
$$\partial_t \mathcal{E} + \operatorname{div}_{\mathbf{x}}((\mathcal{E} + p)\mathbf{u}) = 0,$$

where p refers to the fluid-interface pressure (64).

For sake of completness, we provide the phasic (nonconservative) internal energy equations which read, for k = 1, 2,

(72)
$$\partial_t \left(\alpha_k \rho_k \left(e_k + \frac{|\mathbf{u}|^2}{2} \right) \right) + \operatorname{div}_{\mathbf{x}} \left(\left(\alpha_k \rho_k \left(e_k + \frac{|\mathbf{u}|^2}{2} \right) + \alpha_k p_k \right) \mathbf{u} \right) \\ = \alpha_k p_k \operatorname{div}_{\mathbf{x}} \mathbf{u} - y_k \mathbf{u} \cdot \nabla_{\mathbf{x}} \tilde{p} - p_k \frac{\rho y w}{\sqrt{m}},$$

where $\tilde{p} = p + \frac{m}{2} |\mathbf{D}_t \alpha|^2 + \frac{\nu}{2} |\mathbf{D}_t a_{\mathbf{i}}|^2$.

Now using the transport equations of the specific entropies (42) and the mass conservation equations (41), one deduces that the interfacial entropy complies with

(73)
$$\partial_t(a_i s_i) + \operatorname{div}_{\mathbf{x}}(a_i s_i \mathbf{u}) = 0$$

Then combining (13) and (11) leads to the following interfacial energy evolution equation

(74)
$$\partial_t(a_i e_i) + \operatorname{div}_{\mathbf{x}}(a_i e_i \mathbf{u}) - a_i \gamma_i \nabla_{\mathbf{x}} \cdot \mathbf{u} = \gamma_i \frac{\rho y n}{\sqrt{\nu}}$$

4.1.4. Summary. Using the definitions (67) and (69) the final set of equations reads

(75)
$$\begin{cases} \partial_t \rho + \operatorname{div}_{\mathbf{x}}(\rho \mathbf{u}) = 0, \\ \partial_t(\rho y) + \operatorname{div}_{\mathbf{x}}(\rho y \mathbf{u}) = 0, \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}_{\mathbf{x}}\left(\rho \mathbf{u}^\top \mathbf{u} + \left(p + \frac{m}{2}(\rho y w)^2 + \frac{\nu}{2}(\rho y n)^2\right)\mathbf{Id}\right) = 0, \\ \partial_t \alpha + \mathbf{u} \cdot \nabla_{\mathbf{x}} \alpha = \frac{\rho y w}{\sqrt{m}}, \\ \partial_t a_i + \mathbf{u} \cdot \nabla_{\mathbf{x}} a_i = \frac{\rho y m}{\sqrt{\nu}}, \\ \partial_t w + \mathbf{u} \cdot \nabla_{\mathbf{x}} w = \frac{1}{\sqrt{m}\rho y}(p_1 - p_2), \\ \partial_t n + \mathbf{u} \cdot \nabla_{\mathbf{x}} n = \frac{\gamma_i}{\sqrt{\nu}\rho y}, \\ D_t s = D_t s_1 = D_t s_2 = 0. \end{cases}$$

4.2. Hyperbolicity. To finish we investigate the eigenstructure of the system (75), focusing on its one-dimensional version (with velocity u).

For that purpose, let consider the vector $\hat{\mathbf{B}} = (y, \alpha, a_i, w, n, s, s_1, s_2)^\top \in \mathbb{R}^8$ and write the system (75) in the following quasilinear form

(76)
$$\partial_t \begin{pmatrix} \rho \\ u \\ \hat{\mathbf{B}} \end{pmatrix} + \mathbf{C}(\rho, u, \hat{\mathbf{B}}) \partial_x \begin{pmatrix} \rho \\ u \\ \hat{\mathbf{B}} \end{pmatrix} = \mathbf{R},$$

where $\mathbf{R} = (0, 0, 0, \frac{\rho y w}{\sqrt{m}}, \frac{\rho y n}{\sqrt{\nu}}, \frac{1}{\sqrt{m}\rho y}(p_1 - p_2), \frac{\gamma_i}{\sqrt{\nu}\rho y}, 0, 0, 0)^\top \in \mathbb{R}^{10}$, and the matrix **C** is given by

(77)
$$\mathbf{C}(\rho, u, \hat{\mathbf{B}}) = \begin{pmatrix} u & \rho & \mathbf{0}_{1 \times 8} \\ \frac{\hat{p}}{\partial \rho} & u & \frac{1}{\rho} \nabla_{\hat{\mathbf{B}}} \hat{p} \\ \mathbf{0}_{8 \times 1} & \mathbf{0}_{8 \times 1} & u \mathbf{I}_{8 \times 8} \end{pmatrix},$$

with

$$\hat{p}(\hat{\mathbf{B}}) = \alpha p_1 \left(\frac{\alpha}{y\rho}, s_1\right) + (1-\alpha)p_2 \left(\frac{1-\alpha}{(1-y)\rho}, s_2\right) \\ + \frac{m}{2}(\rho y w)^2 + \frac{\nu}{2}(\rho y n)^2.$$

The eigenvalues of \mathbf{C} are

(78)
$$\lambda_{1,2} = u \pm \rho \sqrt{yc_1^2 + (1-y)c_2^2 + m(yw)^2 + \nu(yn)^2}, \quad \lambda_{3,\dots,10} = u,$$

where $c_k^2 = \frac{\partial p_k}{\partial \rho_k}(\rho_k, s_k)$ is the speed of sound of the phase k = 1, 2. All the eigenvalues are real and the right eigenvectors of **C** constitute a basis of \mathbb{R}^{10} . This proves again the hyperbolicity of the system.

As mention in Remark 1, the SAP depicts reversible processes only. Hence relaxation has to be set *a posteriori* according to the second principle. For instance one may use source terms presented in [17] or [9] to enforce damping due to bubble pulsation. One could also make use of the paragraph 2.3 to design dissipative phase transition source terms in agreement with the thermodynamical equilibrium given in Proposition 2.

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References

- J. Bartak. A study of the rapid depressurization of hot water and the dynamics of vapour bubble generation in superheated water. Int. J. Multiph. Flow, 16(5):789–98, 1990.
- [2] A. Bedford. Hamilton's principle in continuum mechanics. Springer, Cham, [2021] ©2021. doi:10.1007/978-3-030-90306-0.
- [3] Boukili, H. and Hérard, J.-M. Relaxation and simulation of a barotropic three-phase flow model. ESAIM: M2AN, 53(3):1031-1059, 2019. doi:10.1051/m2an/2019001.
- [4] C. Burtea, S. Gavrilyuk, and C. Perrin. Hamilton's principle of stationary action in multiphase flow modeling. working paper or preprint, February 2021. URL: https://hal.science/ hal-03146159.
- [5] H. B. Callen. Thermodynamics and an introduction to thermostatistics, second edition. Wiley and Sons, 1985.

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- [6] P. Cordesse. Contribution to the study of combustion instabilities in cryotechnic rocket engines : coupling diffuse interface models with kinetic-based moment methods for primary atomization simulations. Theses, Université Paris-Saclay, June 2020. URL: https: //theses.hal.science/tel-02948195.
- [7] P. Cordesse, R. Di Battista, Q. Chevalier, L. Matuszewski, T. Ménard, S. Kokh, and M. Massot. A diffuse interface approach for disperse two-phase flows involving dual-scale kinematics of droplet deformation based on geometrical variables. In Second workshop on compressible multiphase flows: derivation, closure laws, thermodynamics, volume 69 of ESAIM Proc. Surveys, pages 24–46. EDP Sci., Les Ulis, 2020. doi:10.1051/proc/202069024.
- [8] P. Cordesse, S. Kokh, R. Di Battista, and M. Massot. Derivation of a two-phase flow model with two-scale kinematics and surface tension by means of variational calculus. In 10th International Conference on Multiphase Flow (ICMF 2019), Rio de Janeiro, Brazil, May 2019. URL: https://hal.archives-ouvertes.fr/hal-02194951.
- [9] R. Di Battista. Towards a unified eulerian modeling framework for two-phase flows : geometrical small scale phenomena and associated flexible computing strategies. Theses, Institut Polytechnique de Paris, September 2021. URL: https://theses.hal.science/tel-03496405.
- [10] F. Drui. Modélisation et simulation Eulériennes des écoulements diphasiques à phases séparées et dispersées : développement d'une modélisation unifiée et de méthodes numériques adaptées au calcul massivement parallèle. Theses, Université Paris-Saclay, July 2017. URL: https://theses.hal.science/tel-01618320.
- [11] D. S. Drumheller and A. Bedford. A thermomechanical theory for reacting immiscible mixtures. Arch. Rational Mech. Anal., 73(3):257–284, 1980. doi:10.1007/BF00282206.
- [12] G. Faccanoni, S. Kokh, and G. Allaire. Modelling and simulation of liquid-vapor phase transition in compressible flows based on thermodynamical equilibrium. ESAIM Math. Model. Numer. Anal., 46(5):1029–1054, 2012. URL: http://dx.doi.org/10.1051/m2an/2011069, doi:10.1051/m2an/2011069.
- [13] G. Faccanoni and H. Mathis. Admissible equations of state for immiscible and miscible mixtures. In Workshop on Compressible Multiphase Flows: derivation, closure laws, thermodynamics, volume 66 of ESAIM Proc. Surveys, pages 1-21. EDP Sci., Les Ulis, 2019. doi:10.1051/proc/201966001.
- [14] S. Gavrilyuk. Multiphase flow modeling via hamilton's principle. In Variational models and methods in solid and fluid mechanics, pages 163–210. Springer, 2011.
- [15] S. Gavrilyuk. 'uncertainty' principle in two fluid-mechanics. ESAIM: ProcS, 69:47-55, 2020. doi:10.1051/proc/202069047.
- [16] S. Gavrilyuk and R. Saurel. Mathematical and numerical modeling of two-phase compressible flows with micro-inertia. J. Comput. Phys., 175(1):326–360, 2002. doi:10.1006/jcph.2001. 6951.
- [17] S. Gavrilyuk and R. Saurel. Mathematical and numerical modeling of two-phase compressible flows with micro-inertia. J. Comput. Phys., 175(1):326-360, 2002. URL: http://dx.doi.org/ 10.1006/jcph.2001.6951.
- [18] J. A. Geurst. Variational principles and two-fluid hydrodynamics of bubbly liquid/gas mixtures. Phys. A, 135(2-3):455–486, 1986. doi:10.1016/0378-4371(86)90154-8.
- [19] H. Gouin. Variational theory of mixtures in continuum mechanics. European J. Mech. B Fluids, 9(5):469–491, 1990.
- [20] H. Gouin and S. Gavrilyuk. Hamilton's principle and Rankine-Hugoniot conditions for general motions of mixtures. *Meccanica*, 34(1):39–47, 1999. doi:10.1023/A:1004370127958.
- [21] P. Helluy and H. Mathis. Pressure laws and fast Legendre transform. Math. Models Methods Appl. Sci., 21(4):745-775, 2011. URL: http://dx.doi.org/10.1142/S0218202511005209, doi:10.1142/S0218202511005209.
- [22] P. Helluy and N. Seguin. Relaxation models of phase transition flows. M2AN Math. Model. Numer. Anal., 40(2):331-352, 2006. URL: http://dx.doi.org/10.1051/m2an:2006015, doi: 10.1051/m2an:2006015.
- [23] M. Hillairet, H. Mathis, and N. Seguin. Analysis of compressible bubbly flows. Part II: Derivation of a macroscopic model. working paper or preprint, March 2022. URL: https: //hal.archives-ouvertes.fr/hal-03621307.
- [24] F. Jaegle, C. Rohde, and C. Zeiler. A multiscale method for compressible liquid-vapor flow with surface tension. ESAIM: Proc., 38:387–408, 2012. doi:10.1051/proc/201238022.

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- [25] A. K. Kapila, R. Menikoff, J. B. Bdzil, S. F. Son, and D. S. Stewart. Two-phase modelling of ddt in granular materials: reduced equations. *Phys. Fluids*, 13:3002–3024, 2001.
- [26] S. Kokh. Lecture notes on stationary action principle applied to fluid problems. Lecture given at the GDR MANU school, Saint Valéry sur Somme, 2016.
- [27] D. Kondepudi and I. Prigogine. Modern Thermodynamics. John Wiley & Sons, Ltd, 2014. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/9781118698723, doi:10.1002/ 9781118698723.
- [28] L. Landau and E. Lifschitz. A Course of theoretical physics, vol 5, Statistical Physics, ch 8. Pergamon Press, 1969.
- [29] D. Lhuillier. Evolution of the volumetric interfacial area in two-phase mixtures. Comptes Rendus Mécanique, 332(2):103-108, 2004. URL: https://www.sciencedirect.com/science/ article/pii/S1631072103002511, doi:https://doi.org/10.1016/j.crme.2003.12.004.
- [30] A. Loison, T. Pichard, S. Kokh, and M. Massot. Two-scale modelling of two-phase flows based on the Stationary Action Principle and a Geometric Method Of Moments. working paper or preprint, 2023. URL: https://hal.science/hal-04188956.
- [31] R. Meignen, B. Raverdy, S. Picchi, and J. Lamome. The challenge of modeling fuel-coolant interaction: Part ii - steam explosion. Nuclear Engineering and Design, 280:528-541, 2014. URL: https://www.sciencedirect.com/science/article/pii/ S0029549314005032, doi:https://doi.org/10.1016/j.nucengdes.2014.08.028.
- [32] F. Smaï. A thermodynamic formulation for multiphase compositional flows in porous media. working paper or preprint, September 2020. URL: https://hal.archives-ouvertes.fr/ hal-02925433.

INSTITUT MONTPELLIÉRAIN ALEXANDER GROTHENDIECK, UNIVERSITÉ DE MONTPELLIER, CNRS, MONTPELLIER, FRANCE

Email address: helene.mathis@umontpellier.fr

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